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14. ABSTRACT
We have developed a methodology that combines computational materials science with statistical learning to rapidly, economically and yet robustly identify key parameters that govern structure-property relationships across length scales. Based on this approach, we have demonstrated, using specific alloy chemistry platforms, practical ways by which information based on designers' needs can be efficiently linked to fundamental materials characteristics. This can provide a strategy for accelerating the identification of promising materials chemistries that will meet the complexity of design parameters. In this manner, expensive and complex experiments and computations need be targeted to only those materials that show the best promise.

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INFORMATICS FOR ALLOY DESIGN

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Abstract

We have developed a methodology that combines computational materials science with statistical learning to rapidly, economically and yet robustly identify key parameters that govern structure-property relationships across length scales. Based on this approach, we have demonstrated, using specific alloy chemistry platforms, practical ways by which information based on designers' needs can be efficiently linked to fundamental materials characteristics. This can provide a strategy for accelerating the identification of promising materials chemistries that will meet the complexity of design parameters. In this manner, expensive and complex experiments and computations need be targeted to only those materials that show the best promise.

Research Summary

The major accomplishments / findings from our research are the following:

a) Discovery of the ability to detect defect structures and lattice distortions from large scale crystallographic data of AB_2 compounds and identify classifications between crystal stoichiometries using data mining techniques. This can provide the basis for new search strategies for designing Laves phases, the largest class of intermetallics and which hold much potential for high temperature structural applications.

b) Discovery of new structure-property correlations in high temperature multicomponent oxides and nitrides that provide a guideline for selecting alloying elements

c) Identification of a new alloy selection design strategy for high temperature alloys. Using this approach we have proposed new ternary alloy additions for binary cobalt based intermetallics. Through comparison with some recent experimental findings reported in the literature, it is suggested that our new findings could serve as a new generation of Co base high temperature alloys that are even better than nickel base superalloys. This strategy has also been extended to the development of new type of design maps that identify targets for Ti alloy chemistries in multicomponent/ multiphase alloys with tailored multifunctional properties.

a) Informatics for binary intermetallic alloy design

This segment of the program explored new ways of classifying potential high temperature binary intermetallics using informatics. Using very large databases, (eg. Linus Pauling File), we have used a combination of Principal Component Analysis (PCA) technique, multiobjective genetic algorithms, and neural networks that evolved through genetic algorithms. The identification of various phases and phase-groups were very successfully done using a decision tree approach (Figure 1)

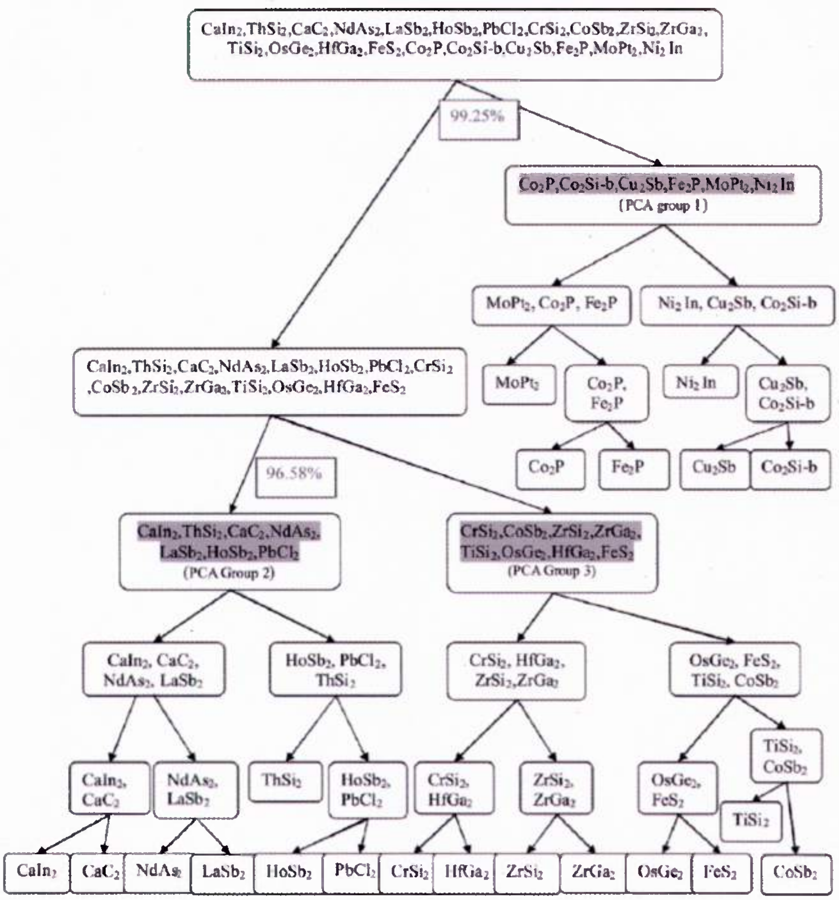
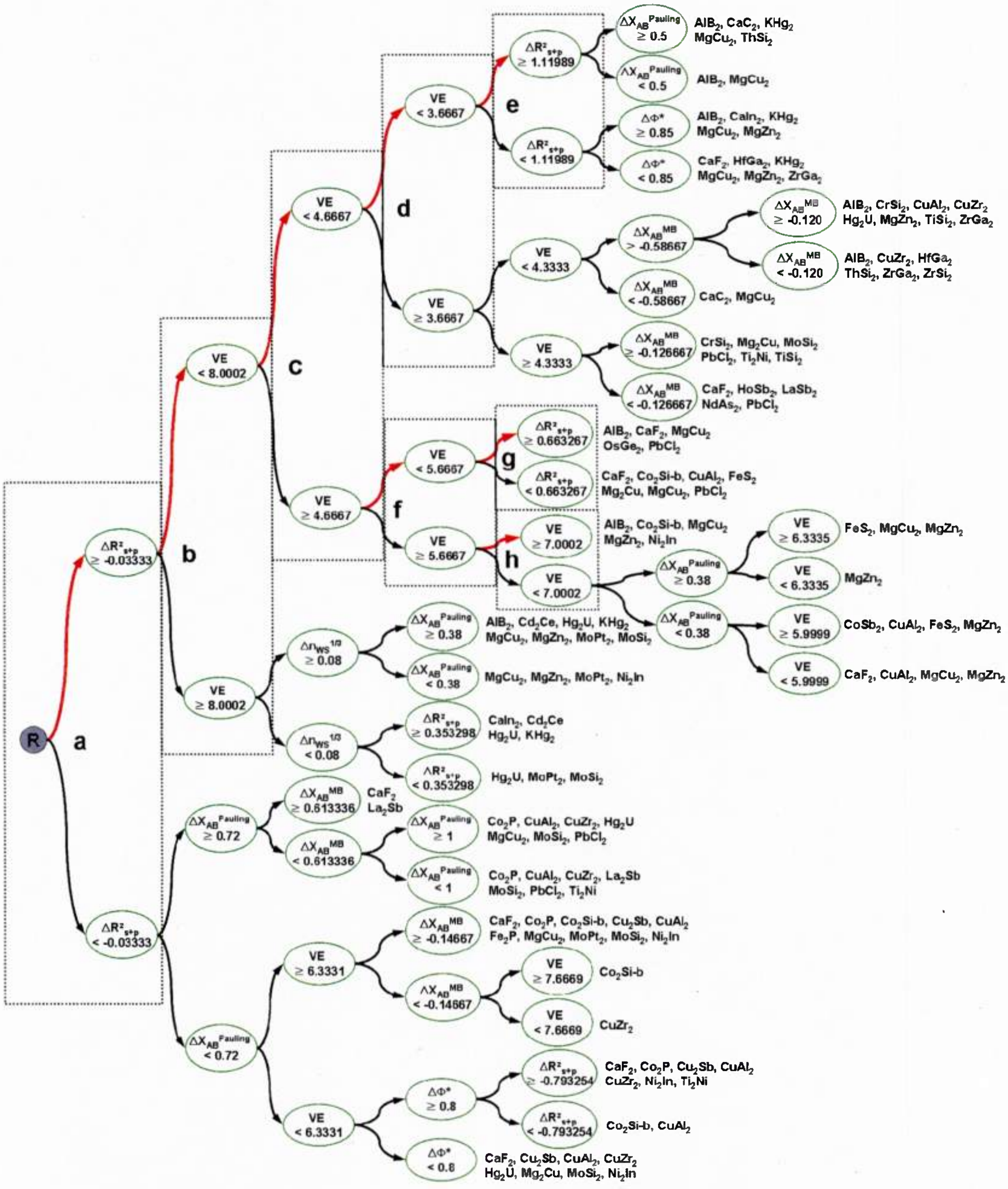


Figure 1: Cu_2Sb in Group 1 falls under the broader class of AB2 compounds dominated by triangular prismatic arrangements, where A resides on 36 nets in paired layer stacking AA. Cu_2Sb is a distortion of a fcc lattice in which there is a displacement of a/2 or b/2 of the ordered atomic array after every two layers along [001], or in which every fourth plane of atoms (Cu) along the [001] is omitted. $CaIn_2$ in Group 2 of the PCA classification is a distorted AlB_2 type structure and part of the class of AB2 structures where the A atoms (e.g., Ca) on triangular nets in a paired layers stacking of AA atoms and the B atoms (In) at half spacings. $CrSi_2$ in Group 3 belongs to a family of polytypic structures AB2 with close packed layers stacked in a bcc sequence (unlike the Group 1 and 2).

Close packed layers are stacked in the [110] bcc stacking sequence with the A (e.g., Cr) atoms of one net lying over the midpoints of the B-B (Si-Si) sides of the triangles of nets above and below. These three examples suggest that the three groupings identified by our combined PCA/GA and neural network approach have effectively managed to classify compounds according to distorted packing sequences. This type of classification via data mining has never been shown before and shows the power of the technique as well as the value of the original set of descriptors used to conduct our data dimensionality reduction analysis. The value of our hybrid data mining approach has been demonstrated by its ability to extract subtle but very important structural classifications that otherwise would not be readily seen simply by examining basic space group information.

In parallel with this new classification analysis, we explored how complex electronic and crystallographic parameters actually govern the stability of intermetallics. This permits us for the first time to develop **design rules** for high temperature intermetallics.

Figure 2: A classification tree for the crystal structures of AB_2 compounds. Using a 28 parameter high dimensional recursive partitioning approach, this tree structure with 29 *if-then* classification rules was achieved. At the terminal nodes, a few (~1-10) crystal structures (prototypes) are suggested as the possible stable structures. Some parts of the tree were highlighted with dot-line boxes to explain the partitioning of parameter space. The pathways indicated by red arrows are juxtaposed with the corresponding parameter-space regions,



We have successfully coupled these design rules to first principles DFT calculations to predict the stability and structure of materials that had yet to be fully characterized.

b) *Informatics for discovering new chemistry-structure relationships of high temperature alloys*

Covalently bonded ceramics such as spinel nitrides are an important class of high temperature materials. Using AB_2N_4 spinel nitrides as a template we have assessed the statistical interdependence of each of a multivariate array of electronic and crystallographic parameters hat that may influence chemistry–structure–property relationships of spinel nitrides. Based on this we have proposed new structure maps for spinel nitrides by identifying the appropriate parameters that have the sensitivity to classify compounds according to the chemistry of site occupancy (Fig. 3)

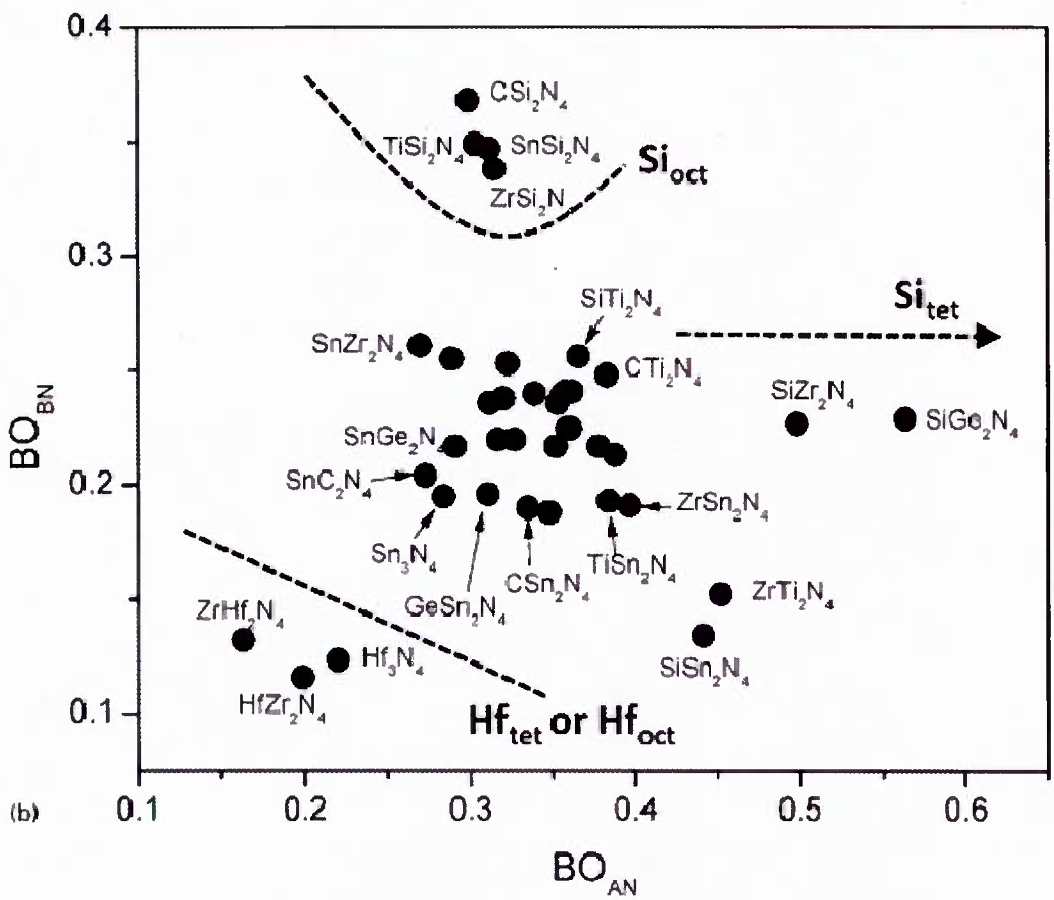


Figure 3 : New classification scheme for high temperature covalently bonded ceramics providing insight into the role of site chemistry and site occupancy on materials stability. This can be used as a guide for both experimental and computational studies in designing new high temperature alloy chemistries.

c) *Informatics for compositional design of multicomponent & multiphase alloys*

We have developed a new method of tracking complex and multidimensional information on the effect of alloy chemistry on the mechanical **properties** of high temperature intermetallic alloys. This has led to the prediction of new cobalt based ternary intermetallic compounds with enhanced high temperature properties compared to conventional nickel based superalloys; and is consistent with empirical observations reported in the literature. The approach involves the use of data dimensionality techniques based on singular value decomposition methods. While such techniques are well established in the data mining and statistical learning community, their use in solving materials science problems is still limited and this project is one of the first to adapt and apply these tools to alloy design. The statistical learning method permits us to discover correlations between dozens of chemical attributes associated with known cobalt based intermetallic alloys based on electronic structure, thermodynamic and property information. From these correlations we have developed formulations that capture the role of chemistry on compounds with targeted properties. This has permitted us to identify which new elements can help alter a known alloy towards a desired property exhibited by another known alloy. By using high dimensional projection methods, we can now develop design "trajectories" that mathematically capture the inference that is normally done in a heuristic manner. We can now propose in an highly accelerated manner, new alloying additions that would not be obvious by just looking at the periodic table. We have

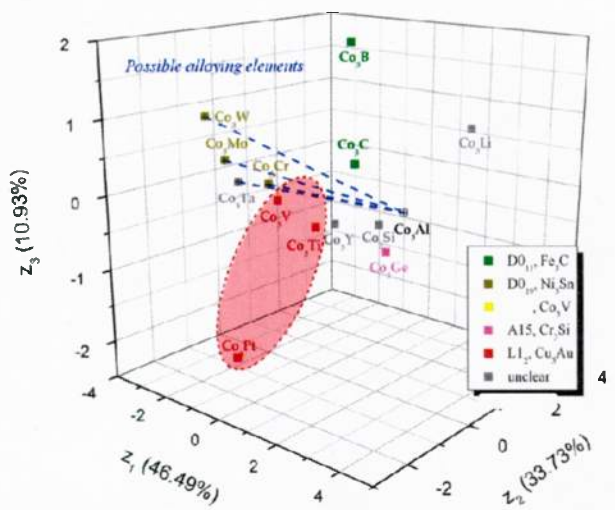


Fig. 4: A new type of design map for high temperature alloys tracking the role of individual alloying elements on properties of binary alloys

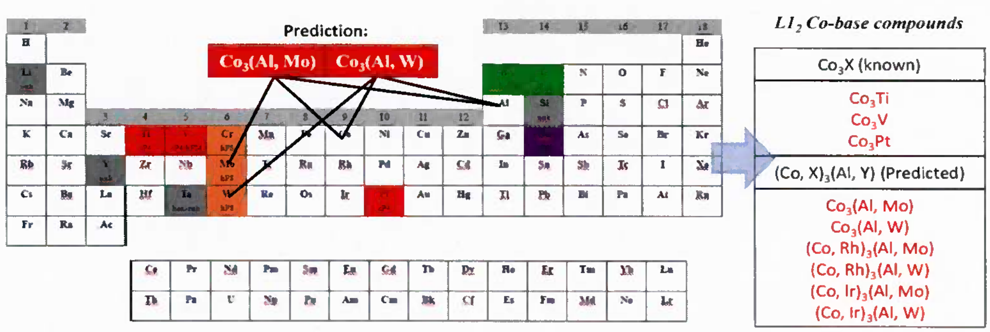


Fig. 5 : Summary of alloying discoveries/ predictions of new ternary cobalt based alloys that can have improved properties from conventional nickel based superalloys.

also extended this work on multicomponent cobalt alloys to *multicomponent-multiphase* Ti alloy design. This ongoing work aims at the prediction of the likely phase relationships and microstructures under different conditions. Figure 5 shows some preliminary results for developing new Ti alloys with desired phase transformation (martensitic transformation from β to α'') and properties (combination of shape memory effect SME and low elastic modulus LEM).

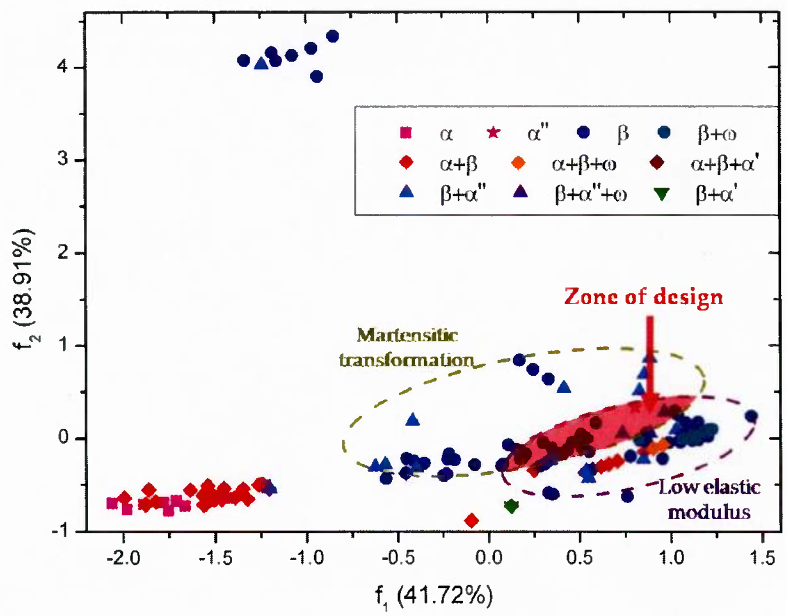


Figure 5 A search space for developing new Ti alloys of desired phases and properties. The plot integrates all possible structural information for Ti alloys, with the axes f_1 and f_2 representing the extracted factors from that information. The dark yellow circle suggests the range for martensitic transformation from β to α'', which brings many interest properties, such as superelasticity and SME. The purple one defines the possible positions for low elastic Ti alloys. Therefore, the overlapping zone (shadow) indicates the coexistence of both properties.

Publications

1. *Materials Informatics parts I and II* : Guest editor: Krishna Rajan: Journal of Metals, Materials & Minerals (JOM) (March 2008 and January 2009)
2. *Materials Informatics:* Guest editors: K. Rajan and P. Mendez: Journal of Statistical Analysis and Data Mining (2009 –in press)
3. *Combinatorial Materials Sciences: Experimental Strategies for Accelerated Knowledge Discovery;* Annual Reviews of Materials Research **38** , 299-322 (August 2008)
4. *Scientific Data Analysis*: C. Kamath, N.Wade, G. Karypis, G. Pandey, V. Kumar, K. Rajan, N.F. Samatova,P. Breimyer, G. Kora, C. Pan and S. Yoginath in Scientific Data Management eds. A. Shoshani and D. Rotem, Taylor and Francis (2008)
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6. *Data Mining and Inorganic Crystallography* Structure and Bonding Series- Springer-Verlag (in press-2009)
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9. *Informatics for Combinatorial Materials Science* : S. Broderick, C.Suh, J. Nowers, B. Vogel, , S. Mallapragada, B. Narasimhan and K. Rajan; Journal of Metals (JOM), 56-59 (March 2008)
10. *Analyzing Sparse Data for Nitride Spinels Using Data Mining, Neural Nets and Multi-objective Genetic Algorithms*: F. Pettersson, C. Suh, H. Saxen, K. Rajan and N. Chakraborti J. Materials and Manufacturing Processes—(2009)
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15. *Materials Genome Project: Data-Mining the Empirical Pseudopotential Method* H. Zenasni, H. Aourag*, S.R. Broderick1, and K. Rajan Physica B- in review
16. "*Designing superlattices for ultra hard coatings: Data mining approach*" by H. Aourag, F. Saidi, S. Broderick, and K. Rajan special issue Physics and Chemistry of Nanoparticles of the Journal of Computational and Theoretical Nanoscience
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18. *Identification and Optimization of AB2 Phases Using Principal ComponentAnalysis, Evolutionary Neural Nets, and Multiobjective Genetic Algorithms* Akash Agarwal a; Frank Pettersson b; Arunima Singh ; Chang Sun Kong ; Henrik Saxén ; Krishna Rajan ;Shuichi Iwata ; Nirupam Chakraborti : Materials and Manufacturing Processes, **24**:3,274 — 281 (2009)

- Manuscripts in preparation:

1. *Informatics based identification of new high temperature cobalt based alloys* : T. Wang and K. Rajan
2. *Informatics based alloy design maps for multiphase titanium alloys*: T. Wang and K. Rajan
3. *Assessment of electronic structure parameters for Ti-Al using data mining:* S. Broderick , H. Aourag and K. Rajan
4. *Information entropy scaled structure map for binary compounds*: C.S. Kong, C. Suh, P. Villars, S. Iwata and K. Rajan

AFOSR Annual Progress Statement Profile Report

Date Published: 09/04/2008

Page One

1. Principal Investigator Name:

KRISHNA RAJAN

2. Grant/Contract Title:

INFORMATICS AIDED ALLOY DESIGN

3. Grant/Contract Number:

FA9550-06-10501

4. Reporting Period Start (MM/DD/YYYY):

July/1/2007

5. End (MM/DD/YYYY):

Aug/31/1008

6. Program Manager

Joan Fuller

7. Annual Accomplishments (200 words maximum):

By combining the alloying theory with data-mining concepts, we have developed an informatics-base strategy for multi-component alloy design. We have developed a strategy for selecting alloying elements for stabilizing L12-structured Co3Al. This strategy has been applied to designing high-temperature Co-base alloys. To find suitable L12-Co3X compounds for Co-base alloy, the formation of various Co3X compounds has been studied by singular value decomposition and similarity analysis techniques. A new type of alloy design map has been developed for identifying possible alloying elements and estimating the relative compositions. We have found Mo and W can be used to stabilize the unstable/ metastable L12-Co3Al, and Co can be replaced by Rh and Ir. A composition formula of Co0.8Al0.1W0.1 was suggested for W stabilized L12-Co3Al, which is in a good agreement with experimental observations. To the best of our knowledge, this is the first time this informatics based approach has been demonstrated to successfully predict new alloy compositions. Work is in progress to expand our approach to other high temperature alloy systems including nickel based superalloys. A set of new hybrid statistical learning techniques have also been developed involved in being be able detect patterns associated with structural distortions among intermetallic crystal structures

8. Archival Publications (published) during reporting period:

1. Data Mining and Informatics for Crystal Chemistry: Establishing measurement techniques for mapping structure-property relationships: - C. Suh and K. Rajan – J. Materials Science and Technology (in press- 2008)

9. Changes in research objectives (if any):

10. Change in AFOSR program manager, if any:

11. Extensions granted or milestones slipped, if any:

12. Attach Report (max. 2MB)

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ANNUAL PROGRESS SUMMARY

To: technicalreports@afosr.af.mil
Subject: Annual Progress Statement to Dr. Joan Fuller

Contract/Grant Title: - Informatics Aided Alloy Design

Contract/Grant #: FA9550-06-10501
Reporting Period: 1 July 2007 to 31 August 2008

Annual accomplishments (200 words max):

By combining the alloying theory with data-mining concepts, we have developed an informatics-base strategy for multi-component alloy design. We have developed a strategy for selecting alloying elements for stabilizing $L1_2$-structured Co_3Al. This strategy has been applied to designing high-temperature Co-base alloys. To find suitable $L1_2$-Co_3X compounds for Co-base alloy, the formation of various Co_3X compounds has been studied by singular value decomposition and similarity analysis techniques. A new type of alloy design map has been developed for identifying possible alloying elements and estimating the relative compositions. We have found Mo and W can be used to stabilize the unstable/metastable $L1_2$-Co_3Al, and Co can be replaced by Rh and Ir. A composition formula of $Co_{0.8}Al_{0.1}W_{0.1}$ was suggested for W stabilized $L1_2$-Co_3Al, which is in a good agreement with experimental observations. To the best of our knowledge, this is the first time this informatics based approach has been demonstrated to successfully predict new alloy compositions. Work is in progress to expand our approach to other high temperature alloy systems including nickel based superalloys. A set of new hybrid statistical learning techniques have also been developed involved in being be able detect patterns associated with structural distortions among intermetallic crystal structures.

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Change in AFOSR program manager, if any: None

Extensions granted or milestones slipped, if any: None

Fuller

DTIC Final Technical Report
Profile Report

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Page One

1. Principal InvestigatorName:

KRISHNA RAJAN

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INFORMATICS AIDED ALLOY DESIGN

3. Grant/Contract Number:

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5. End (MM/DD/YYYY):

10/31/2008

6. Program Manager:

Joan Fuller

7. Distribution Statement (as on SF-298)

Distribution A - Approved for public release

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10. Changes in research objectives (if any):

11. Change in AFOSR program manager, if any:

12. Extensions granted or milestones slipped, if any:

13. Attach Final Report (max. 2MB)(If the report is larger than 2MB, please email file to program manager.)

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